LIMITATIONS OF FULLY IMPLICIT OVERLAND FLOW AND GROUNDWATER MODELS ATTRIBUTABLE TO CONDITIONS OF THE SOLUTION MATRICES

A. M. Wasantha Lal, Naming Wang, M. Z. Moustafa, and Jun Han,
South Florida Water Management District,
3301 Gun Club Rd., West Palm Beach, FL 33406, e-mail: wlal@sfwmd.gov

ABSTRACT

Many large scale overland flow and groundwater flow models such as the MODFLOW model rely on the conservative property of finite volume methods to conserve mass. When implicit finite volume methods and linear equation solvers are used in model formulations, commonly available iterative solution methods referred to as preconditioned conjugate gradient methods or Krylov Subspace methods give reliable mass balance conditions only when the matrix is well conditioned. There is no easy way to look at a model data set and determine if a matrix is ill-conditioned or not. The current paper describes a dimensionless mesh ratio that can be used for this purpose during mesh generations. The paper includes plots of this mesh ratio for a regional model for south Florida. These plots can be useful for deciding the proper mesh size. The results also include estimates of mass residuals corresponding to various mesh ratios.

INTRODUCTION

There are consequences of using very large time steps in models when the parameters and the variables are in extreme ranges. The obvious consequence is instability. The second consequence is the large truncation error resulting from large space and time discretizations. Truncation error has been investigated earlier (Lal, 2000), and is therefore not discussed here. The current paper describes a third consequence which result in large mass balance errors even when conservative numerical methods are applied and implicit solution methods are used to solve them.

The mass residual in a conservative numerical model is the result of poorly conditioned linear equations and the iterative solver packages that are used to solve them. The mass residual is largest when the time step is extremely large and the parameters and the variables fall within certain extreme ranges. With regional hydrologic models, the condition number and the closure criterion can determine the residual in the conservation equation within a model. Even if the mass residual is related to the condition number of a matrix, a dimensionless number referred to as the mesh ratio is introduced in this study as a surrogate for the condition number because it is not easy to obtain the condition number of very large matrices. Unlike the condition number, mesh ratio can be plotted spatially for each cell, and used to evaluate the spatial discretization. The influence of the mesh ratio on the model run time is investigated using MODFLOW (McDonald and Harbough, 1988) and the RSM model (Lal et al., 2005) used in south Florida. A spatial map of the mesh ratio used for the purpose is also shown.

THEORETICAL CONSIDERATIONS

In order to understand the residuals in the equations of mass conservation, the underlying finite volume formulation has to be looked at first. The equation of mass balance in integral form used in the finite volume methods is

$$\frac{\partial}{\partial t}\int_{cv} d\mathcal{V} = -\int_{cs} (\mathbf{E}\cdot\mathbf{n})\, dA \tag{1}$$

This can be written for all the finite volume cells in vector form as

$$\mathbf{A}(\mathbf{H})\cdot\frac{d\mathbf{H}}{dt} = \mathbf{q}\cdot(\mathbf{H}) + \mathbf{S}(\mathbf{H}) \tag{2}$$

in which $\mathbf{H} = [H_1, H_2, \ldots H_m \ldots H_{wb}]^T$ is a vector containing the average heads in the cells; $\mathbf{q}(\mathbf{H}) = [q_1(\mathbf{H}), q_2(\mathbf{H}), \ldots q_{wb}(\mathbf{H})]^T$; $q_i(\mathbf{H})$ = vector containing the net inflow of the cells; $\mathbf{S}(\mathbf{H})$ = the source terms in vector form; $\mathbf{A}(\mathbf{H})$ = a diagonal matrix whose elements A_{mm} are the effective areas of the cells m. This general formulation applies to both the RSM model and the MODFLOW model. The ordinary differential equations (2) are solved by using the following implicit finite difference formulation

$$[\mathbf{A} - \Delta t\mathbf{M}^{n+1}]\cdot\Delta\mathbf{H} = \Delta t[\mathbf{M}^n]\cdot\mathbf{H}^n + \Delta t[\mathbf{S}^{n+1}] \tag{3}$$

Equation 3 is a system of linear equations in the form $\mathbf{P}.\mathbf{x} = \mathbf{b}$ where the right hand side in general represents the net inflow during one time step. The computational procedure begins with the setting up matrix $\mathbf{M}$, which in turn requires the assembly of flow resistance expressions across adjacent cells. Details of the solution of (3) can be found in Lal, (1998), Lal et al, (2005), Akan and Yen, (1981) or McDonald and Harbough, et al. (1988).

The dimensionless mesh ratio B defined here directly relates to the diagonal dominance of matrix $\mathbf{P}$. This can be illustrated using the actual matrix $\mathbf{P}$ itself.

$$B = \frac{m_{ij}\Delta t}{A_i} \tag{4}$$

where m_{ij} is the resistance term between cells or water bodies i and j such that the discharges across them is $m_{ij}(H_i - H_j)$. In the matrix formulation of (3), the condition for diagonal dominance is written as

$$B > B_c \tag{5}$$

where B_c = a critical mesh ratio; $B_c \approx 1/\varepsilon$, and ε = machine precision. For groundwater flow, the mesh ratio described in (4) can be expressed approximately using

$$B_g = \frac{T\Delta t}{s_c A_c}\left(\frac{W}{D}\right) \tag{6}$$

in which, A_c = cell area; W/D = aspect ratio defined as the ratio of the length of the longest cell wall to the height; Δt = time step; T = transmissivity of the aquifer. For unconfined aquifers, $T \approx k\ d$ where $k =$ hydraulic conductivity and $d =$ depth of the aquifer. This equation shows that large A_c values and small values of T and Δt are important for diagonal dominance. For 2-D overland flow models such as RSM, mesh ratio B_o can be defined as

$$B_o = \frac{h^{\frac{5}{3}}\Delta t}{n_b\sqrt{s_n}A_c}\left(\frac{W}{D}\right) \tag{7}$$

When evaluating the residual of implicit finite volume methods, a term residual ratio s used in the following sections is defined as

$$s_{rm} = \frac{\Delta r_o}{|\sum q(H)|\Delta t + |S(H)|\Delta t} \tag{8}$$

where $q(H)$ represents the net inflow of overland and groundwater flow; $\Delta r_o =$ observed volume residual; $S(H) =$ summation of source and sink terms related to rainfall and evapotranspiration (ET).

NUMERICAL EXPERIMENTS

The goal of the first experiment with the RSM model was to find the value of the mesh ratio at the point of breakdown of the mass balance equations. During this experiment, a constant inflow rate was introduced into the model domain with all the outflow boundaries closed. This allowed the water level in the model domain to rise until there was a breakdown in the mass balance equations. This test was carried out with various time steps, Mannings roughness values and cell sizes to generate a wide variety of mesh ratios.

The second experiment involved RSM model implementations over two areas of the Florida Everglades. The first area is cell 4 of the storm water treatment area 1 west (STA1W) managed by the SFWMD. The second area is the nearby Water Conservation Area 2A (WCA2A). During the test, a constant inflow rate was assumed at the marked cell. In order to obtain large mesh ratios for the experiment, an artificial condition was created with a net inflow, zero outflow, and water level rising freely. The mass residual of the cell was calculated as the difference between the inflow volume and the change in storage.

For the experiment with the MODFLOW model, a mesh configuration of five adjacent cells was used for simplicity. An unconfined aquifer of hydraulic conductivity 1000 L/T was assumed for the five square cells of size 100 $L\times$ 100 L. The length and time units were described simply as dimensions L and T because the final results were dimensionless. The storage coefficient was assumed as 0.01. The experiment was conducted with discharge rates $Q =$ 1, 10, 100, 1000, $\cdots 10^6, 10^7\ L^3/T$ applied to the center cell of the five cells. A no-flow boundary was assumed around the flow domain. The water level was allowed to rise during the test. The volume residual was calculated as the difference between the inflow volume and change in volume. The mesh ratio for the problem was calculated using (6). The model was set up to run with the strongly implicit package (SIP), a closure parameter HCLOSE of 0.001, and a maximum number of iterations MAXITER of 120.

RESULTS AND DISCUSSION

Results of the experiment were first used to develop a plot of the mass residual versus the mesh ratio. Figure 1 shows the plot for RSM. In the figure, the log of the mass residual is plotted as a fraction of the net inflow. According to the figure, the mass residual remains generally small and flat until the mesh ratio reaches fairly high values. The scatter in the data is a result of the floating point arithmetic and the truncation error. The figure shows the breaking down of the mass balance equations starting around $B_c \approx 1 \times 10^5$.

Figure 2 shows the mesh ratios obtained from the same experiment have a significant influence on the run time of the RSM model. In presenting these results, the computational effort is used instead of run time so that the results can be used for future applications as well. The computational effort is measured as the number of floating point operations per time step per cell. The figure shows that even with low mesh ratios, the run time increases as the mesh ratio increases. The rate of increase is much faster when the mesh ratio is close to critical values.

Figure 3 shows the mass residuals obtained for the experiment with the MODFLOW model plotted against the mesh ratio. These results can be compared to the results in Figure 1 to show that they are similar. Results of the MODFLOW model show that mass residuals generally remain in the range $10^{-4} \sim 10^{-7}$ and the SIP solver becomes non-convergent when the mesh ratio reaches around 1.0×10^7.

A practical use of mesh ratio is demonstrated using the regional model RSM for the entire south Florida. Figure 4 shows a plot from such an implementation. In this example, plots of mesh ratio were used to detect mesh problems. These mesh ratios were obtained after considering the heterogeneity of the physical properties of the system. The plot shows areas in the mesh with large mesh ratios that need further coarsening. The mesh ratios in the figure can also be used to predict areas in the model that have mass balance issues.

CONCLUSIONS

The study shows the existence of a critical value for the mesh ratio B above which implicit finite volume models do not conserve mass. In the case of RSM, when the number of cells is larger than about 2000, the critical mesh ratio $B_c \approx 10^6$. The study also shows that the mesh ratio can be used as an indicator of potential problems and deficiencies of implicit finite volume models. These deficiencies can include excessive mass residuals, and excessive run times. Even if the condition number is the commonly used indicator for analyzing computational and solver issues, the results show that the mesh ratio is easier to calculate and can be used for the same purpose. The mesh ratio can also be plotted on a map along with other geographic features.

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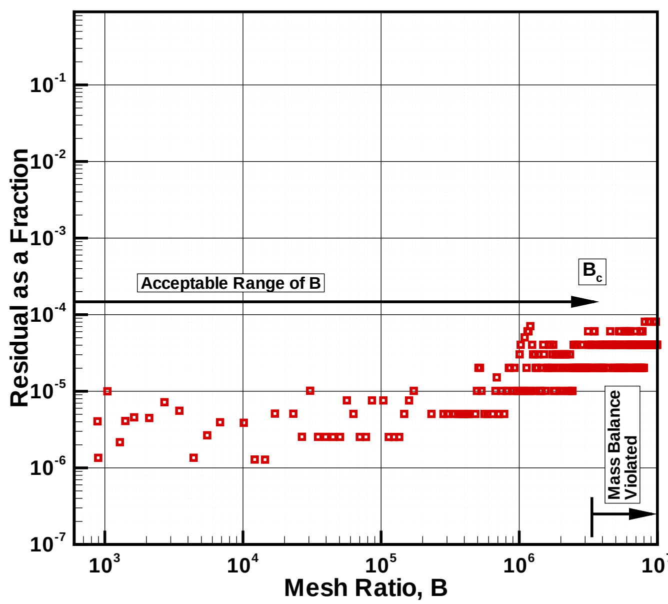

Figure 1: Ranges of residuals as a fraction of net inflow observed for various values of B. The results are obtained from STA1W cell 4 with 202 cells

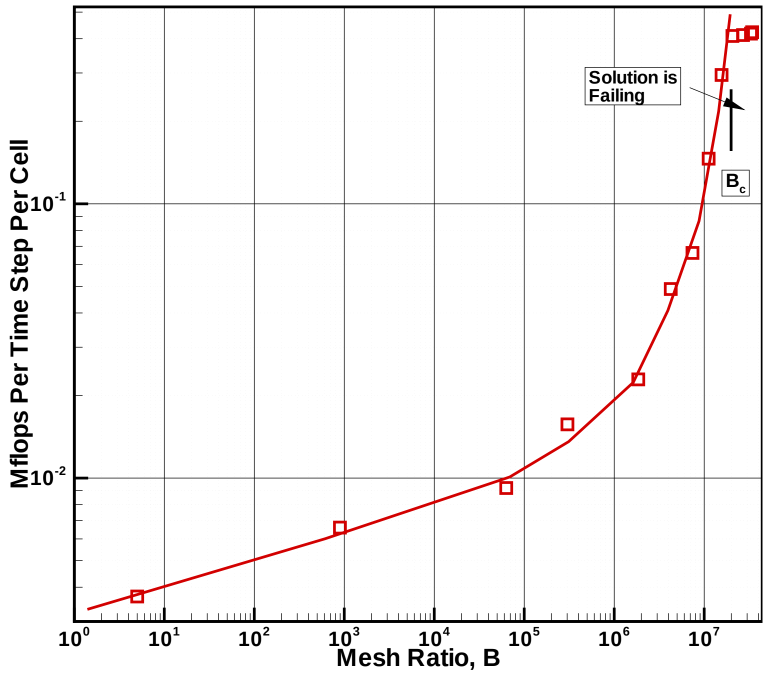

Figure 2: Variation of the computational effort with mesh ratio, B

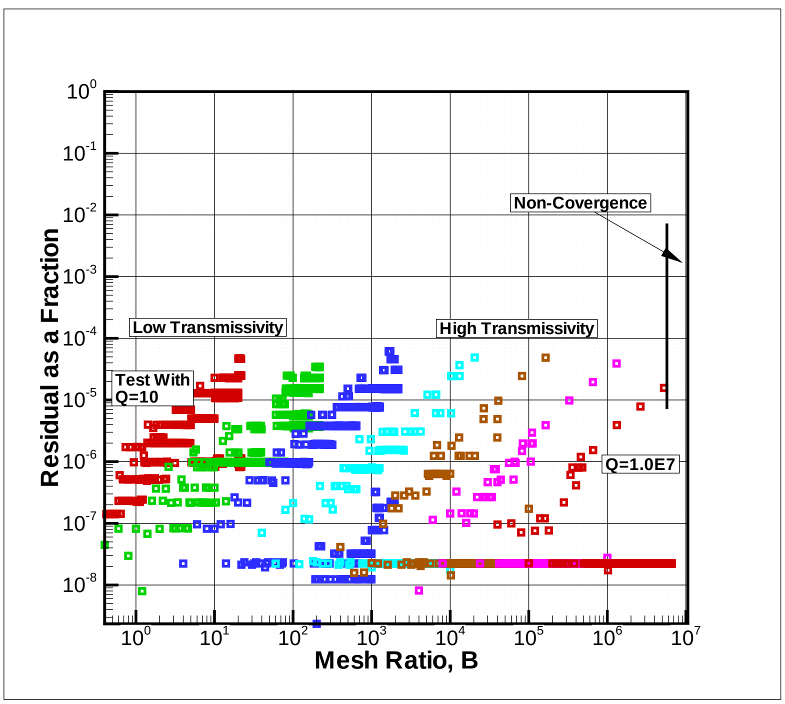

Figure 3: Plot of the mass residual as a fraction of the inflow plotted against the mesh ratio for the MODFLOW model

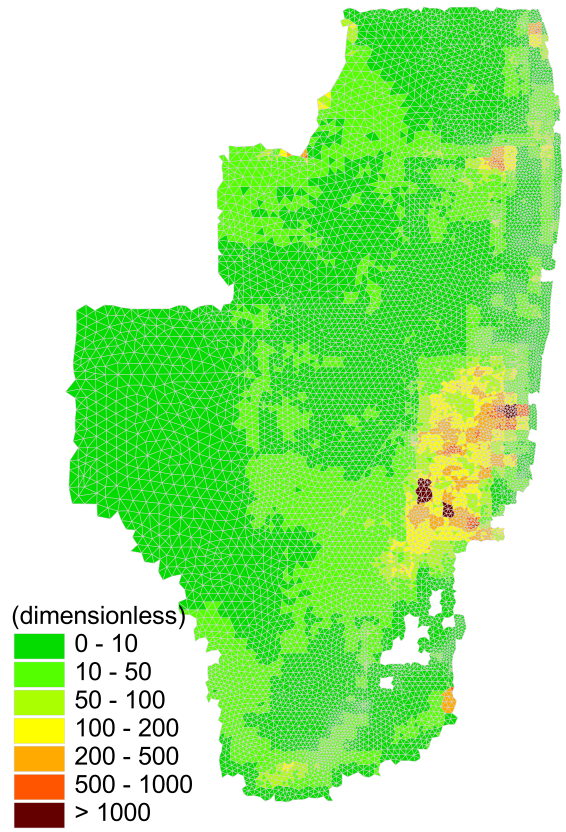

Figure 4: A plot of the mesh ratio of a surface water model for the Florida Everglades. A daily time step is assumed.